Monte Carlo Simulation of a Rarefied Multiphase Plume Flow

Jonathan Burt and Iain D. Boyd
Department of Aerospace Engineering
University of Michigan, Ann Arbor, MI 48109

Exhaust flows from solid propellant rockets are characterized by a number of complex and often overlooked phenomena which should be considered for accurate numerical modeling. In a typical solid rocket motor (SRM), a 10 to 20% mass fraction of aluminum powder is used to reduce combustion instabilities and increase specific impulse. Within the combustion chamber, this aluminum content undergoes a complicated process of melting, heterogeneous combustion, evaporation, agglomeration, and breakup. At the nozzle entrance, a bimodal distribution of liquid alumina (Al_2O_3) droplets exists, made up of agglomerate particles and much smaller smoke particles. As the gas rapidly expands and cools within the nozzle, significant particle velocity and temperature lags develop, both of which are highly dependent on particle size. Combustion, agglomeration and breakup processes may continue through the nozzle and into the nearfield region of the plume. Particle phase change also becomes important in these regions, where heterogeneous crystallization fronts form and progress within supercooled liquid droplets. As a result, complicated distributions of particle size, temperature, number density and velocity often exist in the plume, with a strong dependence on propellant composition, nozzle geometry, combustion chamber pressure, and several other factors[1]. In the performance, contamination or radiation analysis of SRM plume flows, various properties of these alumina particles must be considered, and accurate modeling capabilities are desired for the dominant physical phenomena.

Many of the processes involved have been subject to extensive experimental study, and several CFD-based codes currently exist for the analysis of low to medium altitude SRM plume flows[2]. However, little effort has been devoted to the analysis of such plumes at higher altitudes, where traditional CFD methods often break down due to nonequilibrium characteristics within the gas. In order to avoid the loss of accuracy and stability in CFD modeling of such flows, and to better model rarefaction effects in gas-particle momentum and energy exchange, a project has recently begun to develop and implement techniques for plume flow simulation involving the Direct Simulation Monte Carlo method. This stochastic method has been shown to overcome deficiencies of CFD in the simulation of rarefied plume flows[3], and allows a kinetic theory approach to be used in modeling gas-particle interactions.

A DSMC model for the momentum and energy transfer to a spherical solid particle from a surrounding locally free-molecular monatomic gas has recently been developed by Gallis et al.[4] This model has been extended for two-phase flow simulations involving polyatomic gas mixtures[5], nonspherical particles, and two-way interphase coupling of both momentum and energy[6]. In a paper to be presented soon, the method is further extended to include various effects of solid particle rotation[7]. The current effort involves the development, implementation and evaluation of several additional models, in order to increase accuracy and computational efficiency for the DSMC simulation of high altitude SRM exhaust plumes.

While the DSMC method allows for a high degree of accuracy in the simulation of rarefied gas flows, excessive computational cost is often cited as a major drawback. The same is true for the two-phase model described here; calculations are generally very expensive, so that any improvement in efficiency extends the applicability of the method, as limited resources may be applied to the simulation of larger or more complicated flow domains. With this in mind, a series of coupling parameters are developed to quantitatively evaluate the importance of momentum and energy exchange from the gas to the particles and from the particles to the gas. If interphase coupling in a particular direction and location in the flowfield is determined to have little or no effect on bulk flow characteristics, corresponding calculations for momentum or

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1. REPORT DATE **20 DEC 2004**	2. REPORT TYPE	3. DATES COVERED **-**

4. TITLE AND SUBTITLE **Monte Carlo Simulation of a Rarefied Multiphase Plume Flow**	5a. CONTRACT NUMBER
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) **J Burt; I Boyd**	5d. PROJECT NUMBER **5503**
	5e. TASK NUMBER **000P**
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Air Force Research Laboratory (AFMC),AFRL/PRSA,104 N. Mercury Blvd.,Edwards AFB,CA,93524**	8. PERFORMING ORGANIZATION REPORT NUMBER **AFRL-PR-ED-TP-2004-157**
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Exhaust flows from solid propellant rockets are characterized by a number of complex and often overlooked phenomena which should be considered for accurate numerical modeling. In a typical solid rocket motor (SRM), a 10 to 20% mass fraction of aluminum powder is used to reduce combustion instabilities and increase specific impulse. Within the combustion chamber, this aluminum content undergoes a complicated process of melkting, heretogenous combustion, evaporation, agglomeration, and breakup.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**		**4**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

energy exchange can then be avoided, and the overall numerical efficiency will increase. In the current implementation, four different nondimensional parameters are periodically evaluated in each cell within the DSMC grid, and time-averaged parameter values are compared to set cutoff values to assess the significance of interphase coupling in either direction. These parameters are formulated with the goals of minimizing the cost of parameter evaluations, while allowing for reasonable accuracy over a wide range of flow regimes. Derivations will be provided for all parameters, and a time-averaging scheme used to reduce memory requirements will also be discussed. Further discussion will involve appropriate parameter cutoff values and other issues related to implementation in a DSMC code.

Propulsive efficiency, plume radiation signatures, particle size distributions and other flow characteristics are strongly dependent on the phase composition of particles within the nozzle and plume. Along the nozzle exit plane, the smallest particles are typically made up of some combination of stable α and metastable γ solid phases, while the largest agglomerate particles consist entirely of liquid alumina. Particles of intermediate size may exist as multiphase "slush balls" within the plume nearfield region, where finite-rate crystallization kinetics and steam release allow for combinations of liquid, multiple solid phases, and trapped water vapor within a single particle[2,8]. Phase compositions and phase change processes will have direct and significant effects on the refractive index and the temperature distribution for the particles, as well as several other flow characteristics which may be of interest. Accurate plume simulation therefore requires the consideration of particle phase change, particularly the initial crystallization process for liquid alumina.

A nonequilibrium particle phase change model is implemented in the current code, following ideas of Henderson[9] and Hunter et al.[10] In this model, it is assumed that homogeneous crystallization begins on the surface of a liquid droplet, at a nucleation temperature well below that required for equilibrium melting. A heterogenous crystallization front then progresses toward the particle center, at a velocity which depends on particle velocity but is invariant with radial position. During this process, the particle temperature may either increase or decrease, depending on the balance between convective heat transfer away from the particle and heat release during crystallization. A simple model for particle melting[10] is also implemented, in order to account for any phase change effects associated with particle-shock interactions.

Many authors have suggested that the size distribution of alumina particles within the plume is in large part a result of the breakup or shattering of liquid droplets[11,12]. Previous efforts have focused on modeling breakup within the nozzle, but it seems reasonable to assume that, depending on the flow, particle breakup may be significant well into the nearfield region of the plume. Alumina particle breakup is usually thought to occur as a result of aerodynamic forces on a liquid droplet: The initially spherical droplet begins to deform as surface forces imposed by the gas overcome the restoring effect of surface tension, and eventually the droplet splits into two or more fragments. This process is modeled in the current study following Hunter et al.[10] and Bartlett and Delaney[13], who propose that the critical Weber number at which breakup occurs should be a function of the drag coefficient. Another far less acknowledged but potential significant breakup mode is also considered here. Vasenin et al.[14] have considered the rotation of liquid alumina agglomerates in a nozzle flow, and have postulated that the particle size distribution at the nozzle exit is primarily a result of a centrifugal breakup of rotating droplets. A simple model proposed by these authors has been implemented in the current multiphase DSMC code.

In order to evaluate the physical models and demonstrate capabilities of the code, a simulation is performed on a subscale high altitude SRM exhaust plume flow. Inflow conditions along the nozzle exit plane are based on a CFD nozzle flow simulation. The nozzle geometry is taken from Nelson et al.[15], the particle phase mass fraction and size distribution at the nozzle entrance are based on values given by Anfimov et al.[16], and the gas composition and combustion chamber properties are set such that conditions at the nozzle exit are similar to those found by these same authors. The nozzle flow simulation does not account for effects such as particle phase change, agglomeration, breakup, combustion, or particle-to-gas coupling of momentum or energy, although energy conservation principles are used to approximate the effects of equilibrium crystallization within the nozzle. Note that the nozzle flow simulation is used only to provide generic flow property information at the nozzle exit, so these simplifications can be tolerated with the understanding that the precise modeling of an actual flow is not desired here.

Gas and particle properties along the nozzle exit plane are used to define seven inflow boundaries for an axisymmetric DSMC simulation, which uses a 0.2×0.1 m grid domain consisting of about 26,000 triangular cells. This simulation does incorporate all physical models mentioned above, including two-way coupled momentum and energy transfer between the particles and gas, nonequilibrium phase change, and particle breakup. At steady state approximately 140,000 computational gas molecules and 19,000 solid/liquid particles are simultaneously tracked through the grid. Fig. 1 shows the contours of mass-averaged particle temperature (top) and gas translational temperature. As expected, the particle temperatures are uniformly higher than that of the surrounding gas, with the highest particle temperatures near the central axis where the larger particles are concentrated. Contours of the Sauter mean diameter for the particles is shown in Fig. 2, along with the liquid mass fraction within the particles. The concentration of larger particles toward the axis results in a greater content of liquid alumina within this region, as the reduced surface area-to-mass ratio among larger particles allows for a more gradual process of cooling and solidification.

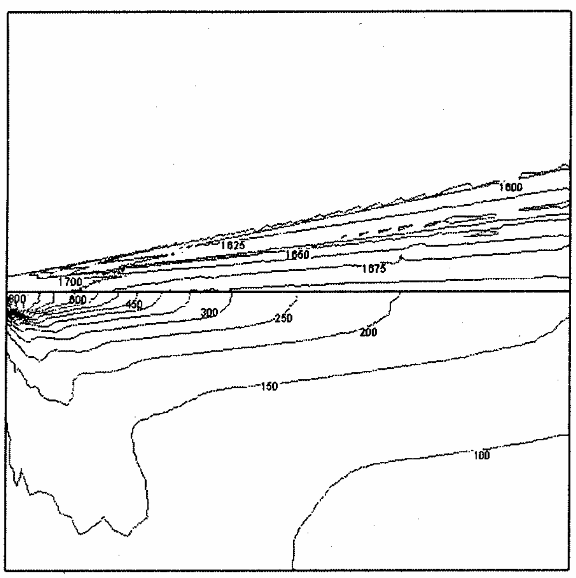

Figure 1. Contours of mass-averaged particle temperature (top) and gas translational temperature. All values are in SI units.

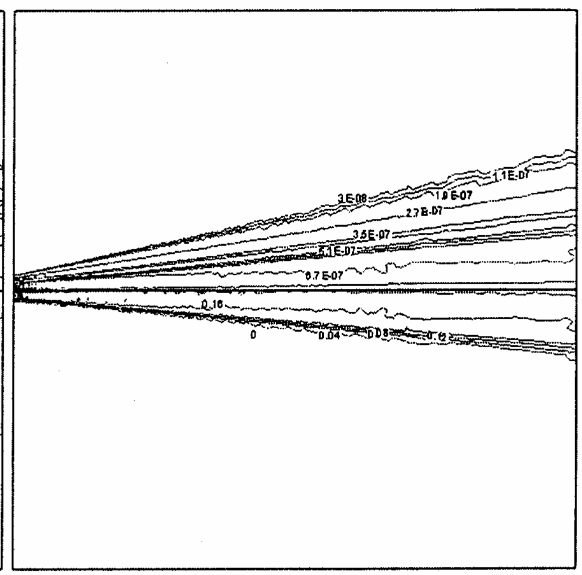
Figure 2. Sauter mean particle diameter (top) and liquid mass fraction of particles.

Additional models are expected to be implemented in the coming months, in order to account for other physical processes which may be important. Radiative heat transfer will be considered, and a detailed model will be developed for use in predicting plume radiation signatures. The code will likely also include models for heterogeneous reactions and particle surface chemistry, evaporation, sublimation, and condensation. Further physical models are also being considered to improve on overall simulation accuracy, and so that multiphase DSMC methods may be applied over a wider range of flow conditions.

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Acknowledgements

The authors gratefully acknowledge the Air Force Research Laboratory at Edwards Air Force Base for financial support of this work, with Dean Wadsworth and Tom Smith as technical monitors.

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